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A new global optimization algorithm hs been developed and applied to molecular structure computation.

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AFOSR 91-0147
Final Technical Report
J.B. Rosen, PI
November 8, 1994

1.   Introduction

The research supported by this grant has produced two important new results during the past 18 months:

1.   A new global optimization algorithm and its application to molecular structure computation.

2.   A generalization of total least squares with important applications to signal processing and parameter estimation. These results are described in two reports (submitted for publication) and one publication. In addition four other papers (based on earlier research supported by this grant) have been published.

The new results are summarized in the next two sections.

2.   Molecular Structure Determination by Convex Global Underestimation of Local Energy Minima.

The determination of a stable molecular structure can often be formulated in terms of calculating the global (or approximate global) minimum of a potential energy function. Computing the global minimum of this function is very difficult because it typically has a very large number of local minima which may grow exponentially with molecule size. The optimization method presented involves collecting a large number of conformers, each attained by finding a local minimum of the potential energy function from a random starting point. The information from these conformers is then used to form a convex quadratic global underestimating function for the potential energy of all known conformers. This underestimator is an $L_1$ approximation to all known local minima, and is obtained by a linear programming formulation and solution. The minimum of this underestimator is used to predict the global minimum for the function, allowing a localized conformer search to be performed based on the predicted minimum. The new set of conformers generated by the localized search serves as the basis for another quadratic underestimation step in an iterative algorithm. This algorithm has been used to determine the structure of n-chain hydrocarbon molecules for $n \leq 22$. While it is estimated that there are $O(3^n)$ local minima for a chain of length n, this method requires $O(n^4)$ computing time on average. It is also shown that the global minimum potential energy values lie on a concave quadratic curve for $n \leq 22$. This important property permits estimation of the minimum energy for larger molecules, and also can be used to accelerate the global minimization algorithm. For a complete description, see [1].

3.    Structure Preserving Total Least Squares Method and Its Application to Parameter Estimation.

A new formulation and algorithm is described for computing the solution to an overdetermined linear system, $Ax = b$, with possible errors in both A and b. This approach preserves the special structure of A, such as Toeplitz or sparse, and minimizes a measure of error in the discrete $L_p$ norm, where p = 1, 2 or $\infty$. It can be considered as generalization of Total Least Squares and we call it Total Least Norm (TLN).

The TLN problem is formulated, the algorithm for its solution is presented and analyzed, and computational results are summarized which illustrate the algorithm convergence and performance on a variety of structured problems. For each test problem, the solutions obtained by least squares, total least squares, and TLN with p=1,2, and $\infty$ were compared. These results confirm that the TLN algorithm is an effective method for solving problems where A or b has a special structure, or where errors can occur only in some of the elements of A and b.

We study the application of the TLN method to various parameter estimation problems in which the perturbation matrix E or [E | r] keeps the Toeplitz structure like the data matrix A or [A | b]. In particular, the $L_2$ norm TLN method is compared with the ordinary LS and TLS method in deconvolution, transfer function modeling and linear prediction problems, and shown to improve the accuracy of the parameter estimates by a factor 2 to 40 at any signal-to-noise ratio. For a complete discussion of this work, see [2, 3].

4.    References and Publications.

1.    J.B. Rosen and A.T. Phillips, Molecular structure determination by convex global underestimation, University of Minnesota Supercomputer Institute (UMSI) Report 94/126. August 1994. Submitted for publication.

2.    J.B. Rosen, H. Park and J. Glick, Total least norm formulation and solution for structured problems, UMSI Report 93/223. November 1993. Submitted for publication.

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4.    A.T. Phillips and J.B. Rosen, Sufficient conditions for solving linearly constrained separable concave global minimization problems, J. of Global Optimization, Vol. 3 (1993), pp. 79-84.

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